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Modeling the dynamics of a changing range genetic algorithm

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Abstract

The paper extends an approach of modeling the dynamics of the genetic algorithm that based on the methods from statistical physics. These methods are applied to describe the effect of an adjustment of a search space size of GA according to a power law on the macroscopic statistical properties of population such as the average fitness and the variance fitness of population. An interaction of the various genetic algorithm operators and how these interactions give rise to optimal parameters values is studied. The equations of motion are derived for the one-max problem that expressed the macroscopic statistical properties of population after reproductive genetic operators and an adjustment of a search space size in terms of those prior to the operation. Predictions of the theory are compared with experiments and are shown to predict the average fitness and the variance fitness of the final population accurately.

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Keywords: genetic algorithms; optimization; statistical mechanics techniques.

1. Introduction

Genetic Algorithm (GA) has become popular tools for search, optimization, machine learning and solving design problem. These algorithms use simulated evolution to search for solutions of a complex problem. A GA is a population-based computational method where the population using randomized processes of selection, crossover, and mutation evolves towards better solutions[1]. To solve efficiently the different complex problems a GA employs a different set of operators that include the common operators of GA like selection, mutation and crossover operators, and the operators which are specific for a particular GA. There are several surveys available[1-5] which discuss in details the implementation of a different set of operators and their advantages and disadvantages.

One way to improve a search strategy is to reduce the search space towards the feasible region where the global optimum is located. These approaches dynamically adjust a search space size and direct GA to the global optimum. These approaches are based on the idea that a parameter-space size adjustment improves accuracy of the discrete sampling in the solution space and significantly reduces the computational time to reach the global optimum[6-10]. Amirjanov[11] analyzed these approaches and employed statistical mechanics techniques to make a mathematical

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modeling of an adjustment of a search space size. The statistical mechanics approach models an ensemble of populations to find an average of some population statistics. The statistical properties of the ensemble won't fluctuate, even though the members of the populations will. According to this approach to model a changing range genetic algorithm (CRGA) the following equations can be derived to take the population of a CRGA from a generation t to a generation t+1:

$$\begin{pmatrix}\mu(t)\\ \sigma(t)\end{pmatrix} \xrightarrow{selection} \begin{pmatrix}\mu_s(t)\\ \sigma_s(t)\end{pmatrix} \xrightarrow{mutation} \begin{pmatrix}\mu_m(t)\\ \sigma_m(t)\end{pmatrix} \xrightarrow{crossover} \begin{pmatrix}\mu_c(t)\\ \sigma_c(t)\end{pmatrix} \xrightarrow{size\,adjustment} \begin{pmatrix}\mu_a(t)\\ \sigma_a(t)\end{pmatrix} = \begin{pmatrix}\mu(t+1)\\ \sigma(t+1)\end{pmatrix} \tag{1.1}$$

In the paper[11] for modeling a GA with dynamical adjustment of a search space size the one-max problem was considered where each site contributed a different amount to the cost of solution. Every individual of population was defined by L binary variables, $x_i \in \{0,1\}$ with weight J_i, and it was mapped to the interval $[u_l, u_u]$, where u_l is a lower bound and u_u is an upper bound of a specified interval. The problem was to optimize a cost function E over the x's,

$$E_\alpha = u_l + (u_u - u_l)\cdot \sum_{i=0}^{L-1} J_i \cdot x_i^\alpha \tag{1.2}$$

where the J_i are fixed weights at each site.

However, the paper[11] focused only on mathematical description of a size adjustment operator by considering for large selection rates and/or large mutation rate that the population converges rapidly towards its asymptotic limit, where the average fitness and the variance fitness are not changeable by selection, mutation and crossover operators.

This paper will focus on deriving the equations that describe the effect of all CRGA's operators on the macroscopic statistical properties of population which change in time. The full dynamics will be calculated by iterating the sequence in (1.1) starting from the initial population.

2. The genetic algorithm model

3. The goal of the modeling is to assess the evolution in the distribution of fitness of population. It means that, for each GA's operator, the distribution of fitness should be calculated after that operator is applied. In this paper we assume that the distribution of fitness is Gaussian[12]. As a result it is sufficient to consider only $\mu(t)$ and $\sigma^2(t)$.

3.1. Selection dynamics

Selection is the operation whereby more fit strings are increased in the population at the expense of less fit ones. The effect of selection on the distribution of phenotypes within the population is independent of the genotype to phenotype mapping for a particular problem. This is a consequence of the fitness being a function of the phenotype only. It is therefore possible to model selection without reference to a specific problem.

The binary tournament selection is used as a GA selection operator in this paper. In binary tournament selection two members are randomly drawn from the population and the fitter member is copied into the mating pool. Blickle and Thiele[13] obtained the following expressions for infinite population to assess the effect of selection on the average and the variance fitness of population:

$$\mu_s = \mu + \frac{\sigma}{\sqrt{\pi}} \tag{2.1}$$

$$\sigma_s^2 = \left(1 - \frac{1}{\pi}\right)\cdot \sigma^2 \tag{2.2}$$

4. The expressions (2.1, 2.2) were obtained for an infinite population. However, the macroscopic properties of any finite population drawn from the ensemble will differ slightly due to well-known sampling effects[12]. It can be seen that the mean is unchanged, but the variance of a finite population is reduced. Because of a finite population correction the formulae (2.1, 2.2) can be rewritten as follows:

$$\mu_s = \mu + \frac{\sigma}{\sqrt{\pi}} \tag{2.3}$$

$$\sigma_s^2 = \left(1-\frac{1}{\pi}\right)\cdot\left(1-\frac{1}{P}\right)\cdot\sigma^2 \tag{2.4}$$

The increase in the mean is proportional to the variance in the population, and the variance is reduced through finite population sampling.

4.1. Mutation dynamics

5. Mutation operator alters a string locally to hopefully create a better string. Mutation acts on each member of the population independently. The effect of mutation (and crossover) on a string will not depend only on the fitness distribution, it will also depend on the configuration of strings. Mutation operator *m* changes a site *I* of a string α with probability p_m, that is[14]

$$m_i^\alpha = \begin{cases} x_i^\alpha & \text{with probability } 1-p_m \\ 1-x_i^\alpha & \text{with probability } p_m \end{cases} \tag{2.5}$$

To calculate the average effect of mutation on a site of the string α we need to average overall possible mutations. Denoting the average overall possible mutations by $\langle\cdots\rangle_m$ the following can be obtained:

$$\left\langle x_i^{m\alpha}\right\rangle_m = (1-p_m)\cdot x_i^\alpha + p_m\cdot(1-x_i^\alpha) = p_m + (1-2\cdot p_m)\cdot x_i^\alpha \tag{2.6}$$

The average fitness of a string after mutation can be calculated by combining the expressions (1.2) and (2.6). For the weights $J_i = \frac{2^i}{2^L-1}$ which represents a conversion of a binary code to a decimal code the last formula can be simplified as follows:

$$\mu_m = p_m\cdot(u_u+u_l) + (1-2\cdot p_m)\cdot\mu \tag{2.7}$$

The variance of the population after mutation can be calculated similarly by averaging a variance of a string over all members of population and all mutations.

$$\sigma_m^2 = p_m\cdot(1-p_m)\cdot(u_u-u_l)^2\cdot\sum_{i=0}^{L-1}J_i^2 + (1-2\cdot p_m)^2\cdot\sigma^2 \tag{2.8}$$

The formula (2.8) should be corrected by coefficient $(1-1/P)$ because of a sampling effect of a finite population, like it was done for selection operator. If $J_i = \frac{2^i}{2^L-1}$, which represents a conversion of a binary code to a decimal code, then

$$\sigma_m^2 = \left(1-\frac{1}{P}\right)\cdot\left(p_m\cdot(1-p_m)\cdot(u_u-u_l)^2\cdot\frac{2^L+1}{3\cdot(2^L-1)} + (1-2\cdot p_m)^2\cdot\sigma^2\right) \tag{2.9}$$

The observation of (2.7) and (2.9) shows that the average and the variance fitness of population after mutation can be expressed in terms of the same properties of population before mutation.

5.1. Crossover dynamics

Crossover operator allows the mixing of parental information when it is passed to their offspring. The result of crossover is a randomized exchange of genetic material between individuals with the possibility that good solutions can generate even better ones. Like mutation the effects of crossover depends on the configurations of strings as well as the fitness distribution. There are many possible crossover schemes available and which is most appropriate depends on the problem under consideration[1]. The simplest to calculate is "uniform crossover" where a child is constructed from its two parents by choosing each site at random from either of the parents[12].

For a uniform crossover, the alleles of a child γ produced by parents α and β are given in[15],

$$x_i^\gamma = \mathrm{X}_i^{\alpha\beta}\cdot x_i^\alpha + (1-\mathrm{X}_i^{\alpha\beta})\cdot x_i^\beta, \quad \text{where} \quad \mathrm{X}_i^{\alpha\beta} = \begin{cases} 1 & \text{with probability } p_c \\ 0 & \text{with probability } 1-p_c \end{cases} \tag{2.10}$$

where p_c is a probability of crossover.

Prügel-Bennett and Shapiro[12] showed that with reasonable approximation a uniform crossover leaves the average fitness and the variance fitness of population unchanged, that is

$$\mu_c \approx \mu \tag{2.11}$$

$$\sigma_c^2 \approx \left(1-\frac{1}{P}\right)\cdot\sigma^2 \tag{2.12}$$

In fact, a crossover involves the interaction of different population members which can be measured by a correlation between the sites of two members. The correlation is a measure of the microscopic similarity of genotypes of population members. The changing of the mean correlation within the population indicates the changing of distribution of population, and, consequently, the macroscopic statistical properties of population. However, the mean correlation is unchanged by crossover, because although crossover changes the alleles within each population member, it conserves the mean number of alleles at each site within the population[15].

5.2. Dynamics of an adjustment of a search space size

To model an effect of an adjustment of a search space size (adjustment operation) on the macroscopic statistical properties a law of a changing range of a mapped interval should be established. In paper[11] a power law was used for a changing range of a mapped interval that is

$$(u_{ua}-u_{la}) = (u_{u0}-u_{l0})\cdot k^t \tag{2.13}$$

where u_{la} and u_{ua} are a lower and an upper bounds respectively after the adjustment operation, u_{l0} and u_{u0} are the initial lower and an upper bounds, and t is a number of generations.

The new mapped interval is centered on the average fitness of population[11]. Thus, according to (2.13) the following expressions can be established for calculating the lower and upper bounds of the new mapped interval:

$$u_{la} = \begin{cases} u_{l0} & \text{, if } u_{la} \le u_{l0} \\ \mu-(u_{u0}-u_{l0})\cdot k^t/2, & \text{otherwise} \end{cases} \tag{2.14}$$

$$u_{ua} = \begin{cases} u_{u0} & \text{, if } u_{ua} \ge u_{u0} \\ \mu+(u_{u0}-u_{l0})\cdot k^t/2, & \text{otherwise} \end{cases} \tag{2.15}$$

Denoting the average over all individuals of the population by $\langle\cdots\rangle$ the average fitness μ_a after the adjustment operation can be expressed as follows:

$$\mu_a = \langle E_\alpha^a\rangle_\alpha = u_{la} + (u_{ua}-u_{la})\cdot\sum_{i=0}^{L-1} J_i\cdot\langle x_i\rangle_\alpha \tag{2.16}$$

The average fitness of population in genotype space denoted by $\langle x_i\rangle_\alpha$ is not changed after the adjustment

$$\mu_a = u_{la} + (u_{ua}-u_{la})\cdot\frac{\mu-u_l}{u_u-u_l} \tag{2.17}$$

where u_l and u_u are a lower and an upper bounds respectively before the adjustment operation. The variance σ_a^2 after the adjustment operation can be expressed in term of the variance σ^2 before the operation as follows:

$$\sigma_a^2 = \left\langle\left(E_\alpha^a-\mu_a\right)^2\right\rangle_\alpha = \left(\frac{u_{ua}-u_{la}}{u_u-u_l}\right)^2\cdot\sigma^2 \tag{2.18}$$

6. Modeling the full dynamics

For modeling the full dynamics of the GA according to (1.1) the iteration process of calculating macroscopic statistical properties of population should be applied. It means that the changes of the macroscopic statistical properties of population caused by selection, mutation, crossover and size adjustment operators need to be computed. It can be done by applying the equations (2.3, 2.4) to initial population for modeling the selection operator, then by applying the equations (2.7, 2.9) to model the mutation operator, then by applying the equations (2.11, 2.12) to model the crossover operator, and last by applying the equations (2.17, 2.18) to model the adjustment

operator. Before calculating the equations (2.17, 2.18) the lower and upper bounds of the size space need to be calculated by using the equations (2.14, 2.15). This procedure is then iterated an arbitrary number of generations to get from the initial distribution to the final one.

For modeling the full dynamics of the GA the initial macroscopic statistical properties of population should be calculated. The initial strings are generated by randomly setting each site to 0 or 1 with probability 0.5. The equations for mutation (2.7, 2.9) can be used to compute the initial macroscopic statistical properties of population. Putting $p_m = 0.5$ in equations (2.7) and (2.9) gives for the initial average fitness (μ_0) and the initial variance fitness of population (σ_0^2) the following expressions:

$$\mu_0 = 0.5 \cdot (u_{u0} + u_{l0}) \tag{3.1}$$

$$\sigma_0^2 = \left(1 - \frac{1}{P}\right) \cdot \frac{2^L + 1}{12 \cdot (2^L - 1)} \cdot (u_{u0} - u_{l0})^2 \approx \left(1 - \frac{1}{P}\right) \cdot \frac{(u_{u0} - u_{l0})^2}{12} \tag{3.2}$$

The result of computing the changes of the average fitness (μ) and the standard deviation (σ) of population caused by selection, mutation, crossover and size adjustment operators over 50 generations starting from initial population is shown in Fig. 1. Fig. 1 represents a comparison between the theory (solid line) and simulations (dashed line) averaged over 6000 runs.

Analysis of the curves in Fig. 1 shows that the theoretical model accurately enough predicts the behaviour of a GA, although there are clearly systematic errors in the predictions of the theory. This discrepancy arises from a number of assumptions made to capture the full dynamics of the GA, but not at the expense of an over complex model. The first assumption made was that the distribution of fitness is Gaussian. As a result only $\mu(t)$ and $\sigma(t)$ were considered.

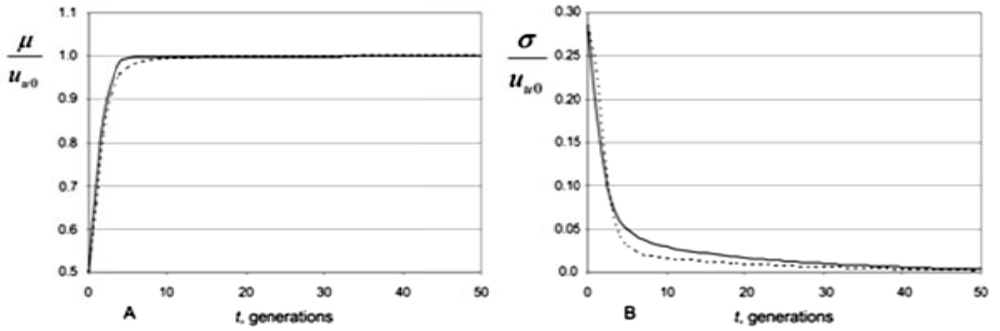

Fig. 1. Simulation (dashed line) and theory (solid line) for A) the average fitness and B) the standard deviation. The curves are for $P = 50$, $L = 100$, $p_m = 0.01$, $p_c = 0.65$ and $k = 0.95$. The simulations are averaged over 6000 runs.

This assumption in the number of macroscopic variables is significant as it enables closed form expressions to be derived for the evolution dynamics. The other source of error is in sample-to-sample fluctuations. The transformation which predicts the macroscopic statistical properties at a given time in terms of those in the previous time is nonlinear. Although the macroscopic statistical properties are self-averaging quantities of which sample-to-sample fluctuations should be small, nonlinear functions of the properties are not necessarily self-averaging[12].

An influence of a coefficient of reduction of a mapped interval k on the macroscopic statistical properties of population ($\mu(t)$ and $\sigma(t)$) is shown in Fig. 2. Fig. 2 represents only the results of simulations. It is clear from Fig. 2 that with the adjustment operation the average fitness of population at the end of the run is significantly closer to the maximum than without an adjustment of a search space size. It can be seen that the curve without an adjustment of a search space size and all curves with any level of a coefficient k have almost the same transient period to reach an equilibrium point (the vertical dashed lines). At an equilibrium point the improvement due to selection is balanced by a loss of fitness caused by mutation and crossover operators. At that point the population becomes homogeneous. From that point the improvement of the average fitness of population will be made only by the

adjustment operator. The adjustment operator does not change the average fitness and the standard deviation of population in genotype space (a diversity of population) which is proved by the expressions (2.16, 2.18), but moves the population to the maximum by tightening a search space size.

For assessment of the transient period to reach an equilibrium point the model that consists of mutation, selection and crossover operators can be considered. Applying the selection (2.3, 2.4), mutation (2.7, 2.9) and crossover (2.11, 2.12) operators together produces the following expressions for the average fitness and the variance fitness of population:

$$\mu(t+1) = p_m \cdot (u_u + u_l) + (1 - 2 \cdot p_m) \cdot \left(\mu(t) + \frac{\sigma(t)}{\sqrt{\pi}} \right) \tag{3.3}$$

$$\sigma^2(t+1) = \frac{1}{3} \cdot p_m \cdot (1 - p_m) \cdot (u_u - u_l)^2 \cdot \left(1 - \frac{1}{P}\right) + (1 - 2 \cdot p_m)^2 \cdot \left(1 - \frac{1}{\pi}\right) \cdot \left(1 - \frac{1}{P}\right)^3 \cdot \sigma^2(t) \tag{3.4}$$

The solution of the system equation above with $p_m << 1$ at equilibrium is

$$\mu(t_\mu) \approx \mu(\infty) \approx \frac{(u_u + u_l) \cdot \left(p_m + \sqrt{p_m/3}\right)}{2 \cdot p_m} \tag{3.5}$$

$$\sigma^2(t_{\sigma^2}) \approx \sigma^2(\infty) \approx \frac{\pi \cdot p_m \cdot (u_u - u_l)^2}{3} \tag{3.6}$$

where t_{σ^2} is a transient period of the variance to converge to its equilibrium value and t_μ is a transient period of the average fitness to converge to its equilibrium value.

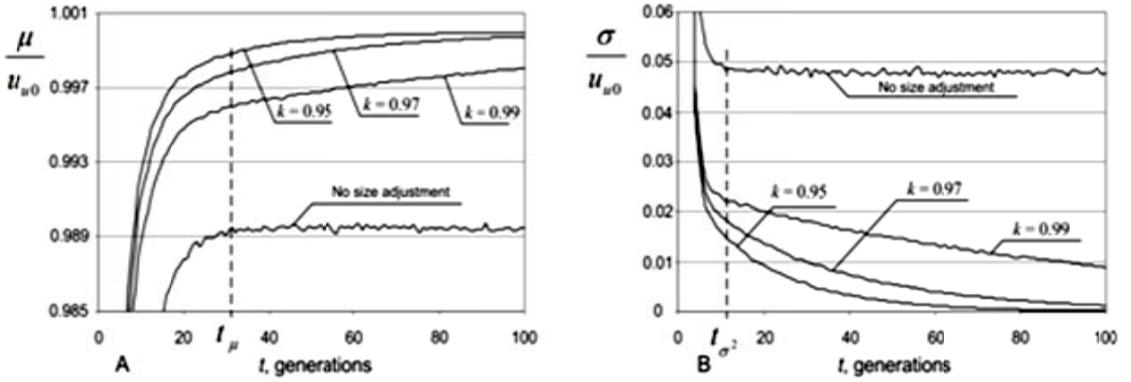

Fig. 2. Simulations for A) the average fitness and B) the standard deviation with different values of coefficient k. The curves are for P = 50, L = 100, p_m = 0.01, p_c = 0.65. The simulations are averaged over 6000 runs.

The characteristic time decay is $\tau_{\sigma^2} = -\log((1 - 2 \cdot p_m)^2 \cdot (1 - 1/\pi))$ at which $\sigma^2(t)$ converges to its equilibrium value. This convergence rate depends on two factors: the convergence due to mutation and the convergence due to selection, and it does not depend on the size of a search space. But an equilibrium value of the variance depends on a size of a search space; the reduction of a search space size diminishes the variance fitness of population (see 3.6).

The characteristic time decay at which $\mu(t)$ converges to its equilibrium value is $\tau_\mu = -\log(1 - 2 \cdot p_m)$. The convergence of $\mu(t)$ is slower. It converges first through the variance and then converges at a rate τ_μ which is controlled by the mutation rate alone. The convergence rate of the average fitness does not depend on the size of a search space, but its equilibrium value depends on it; the reduction of a search space size increases the average fitness of population for the first scenario[11].

From the equilibrium point the average fitness of population continues to increase (see Fig. 2), but now only because of the adjustment operator. It means that the adjustment operator follows the first scenario by incrementing

a lower bound, and fixing an upper bound of a mapped interval to u_{u0} because $u_{ua} > u_{u0}$, that is (see 2.16)

$$\sum_{i=0}^{L-1} J_i \cdot \langle x_i \rangle_\alpha = \frac{\mu(t_\mu) - u_l(t_\mu)}{u_{u0} - u_l(t_\mu)} = C \tag{3.7}$$

C is a constant up to the end of the run, because only the adjustment operator is operational, and it does not change the average fitness of population in genotype space denoted by $\langle x_i \rangle_\alpha$. The equation (2.17) that expresses the average fitness of population after the adjustment operator can be rewritten as follows

$$\mu(t) = u_{u0} \cdot C + u_l(t) \cdot (1 - C) \tag{3.8}$$

By moving an origin for *t* (a number of generations) to the equilibrium point and replacing $u_l(t)$ in (3.8) by expression (2.14) the average fitness of population can be obtained

$$\mu(t) = (1 - C) \cdot \mu(t-1) + C \cdot u_{u0} - \frac{u_{u0} \cdot (1 - C)}{2} \cdot k^t \tag{3.9}$$

with the following solution:

$$\mu(t) = \mu(t_\mu) \cdot (1 - C)^t + C_1 + C_2 \cdot k^t \tag{3.10}$$

where $C_1 = u_{u0}$ and $C_2 = \frac{u_{u0} \cdot k \cdot (1 - C)}{2 \cdot (1 - k - C)}$.

Analysis of solution (3.10) shows that after a few generations (*t*) the term $\mu(t_\mu) \cdot (1 - C)^t \approx 0$, because (1-*C*) < 0.5 for the first scenario. It means that the average fitness of population μ for the first scenario will reach the maximum with a characteristic time decay $\tau_\mu = -\log k$, and it comes to an upper bound of the mapped interval, that is $\mu \to u_{u0}$ for $t \to \infty$. Analysis of the expression (3.10) shows that average fitness of population μ depends on a coefficient of shrinking of a mapped interval size k. A decrementing of a coefficient k reduces a number of generations to reach the maximum average fitness of population, but at the same time it reduces a level of the maximum which can be reached by GA. Comparisons of simulation results with theory prediction for the maximal level of the average fitness of the population show that the discrepancies with any level of a coefficient k do not exceed 1%. The variance fitness of population (or the standard deviation of fitness) is reduced according to the expression [11]:

$$\sigma(t) = \sigma(t_\mu) \cdot \left(a^t + \frac{k \cdot (k^t - a^t)}{2 \cdot (k - a)} \right) \tag{3.11}$$

where $a = 1 - \frac{\mu(t_\mu)}{u_{u0}}$. The variance fitness of population reaches a zero for $t \to \infty$.

7. Conclusion

The paper modeled the dynamics of GA with an adjustment of a search space size for one-max problem that follows a power law and derived the equations that describe the effect of GA's operators on the macroscopic statistical properties of the population, such as an average fitness and a variance fitness of population.

The formalism described for modeling of GA with an adjustment of a search space size assumes that the environment and the population form a unique system. The genetic operators (selection, mutation, and crossover) move the population to the region where the maximum is located, and at the same time parameter-space size is adaptively reduced, which is based on idea that the shrinking of the solution space can help to obtain better and accurate fitness value by individuals of population.

It was shown that the conventional GA's operators (selection, mutation and crossover) drive the population to the equilibrium point where the improvement due to selection is balanced by a loss of fitness caused by mutation and crossover operators. A number of generations (a transient period) to reach that point depends on the selection rate and the mutation rate of GA, but does not depend on a coefficient of reduction of a search space size k. However, a

coefficient k influences the levels of the macroscopic statistical properties of population obtained at the end of the transient period. At the end of the transient period the population becomes homogeneous which means that the conventional GA's operators do not change the macroscopic statistical properties of population, and only the adjustment operator continues to drive the population to the maximum. A coefficient of shrinking k exponentially changes the macroscopic statistical properties of population and significantly influences on the computational cost. It was shown that a coefficient k is a trade-off procedure: for reduction of a computational cost the value of k should be reduced, but to obtain a better optimum the value of k should be increased.

The derived equations that express the effect of GA's operators on the macroscopic statistical properties of the population showed that the theoretical model accurately enough predicts the behavior of GA, although there are clearly systematic errors in the predictions of the theory. This discrepancy arises from a number of assumptions made to capture the full dynamics of GA.

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